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BROWNIAN DYNAMICS SIMULATIONS WITHOUT GAUSSIAN RANDOM NUMBERS

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We point out that in a Brownian dynamics simulation it is justified to use arbitrary distribution functions of random numbers if the moments exhibit the correct limiting behavior prescribed by the Fokker–Planck equation. Our argument is supported by a simple analytical consideration and some numerical examples: We simulate the Wiener process, the Ornstein–Uhlenbeck process and the diffusion in a Φ^4 potential, using both Gaussian and uniform random numbers. In these examples, the rate of convergence of the mean first exit time is found to be nearly identical for both types of random numbers.

Keywords: Brownian Dynamics; Numerical Simulation; Random Numbers; Langevin Equations; Stochastic Processes.

1. Introduction

In many branches of physics, and other sciences, the dynamical behavior of various model systems is described by a Markov process continuous in time. Very frequently, processes of the Fokker–Planck type are considered.[1,2] A convenient method to solve a Fokker–Planck equation is the numerical Brownian dynamics simulation. In this method, one exploits the equivalence of the Fokker–Planck equation to a stochastic differential equation, the Langevin equation. In a discretized approximation with finite timestep h, the appearing noise term can be simulated by random numbers. The method then can be viewed as the generation of an ensemble of stochastic trajectories ("paths"). By averaging over these paths, one obtains information about single–time statistical averages $\langle A(t)\rangle$ as well as multi–time correlation functions $\langle A(t)B(t')\rangle$, $\langle A(t)B(t')C(t'')\rangle$, ...

In this note we consider the choice of the distribution function of the random numbers used in a Brownian dynamics simulation. Most simulations up to now have been using normally distributed random numbers. In a recent paper, Greiner, Strittmatter and Honerkamp[3,4] described various discretization schemes for stochastic differential equations and discussed the involved discretization error.

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They pointed out that in the case of the simple Euler algorithm the order of the discretization error of quantities of the type $\langle A(t)\rangle$ remains unchanged if one replaces the Gaussian distribution function by some other distribution function having the same mean and variance and finite higher moments. So, one can use the computationally less expensive uniformly distributed random numbers to calculate $\langle A(t)\rangle$. However, it was not noticed there that *every* statistical property, *including* correlation functions and mean first exit times, is still correctly simulated in the limit $h \to 0$ after the above mentioned replacement. This is, however, a direct consequence of the very definition of a Fokker–Planck process, as will become clear in the following sections. At least according to our knowledge of the pertaining literature, most authors who have applied the method seem to be unaware of this fact. Our communication, therefore, hopes to demonstrate to the practitioner in the field that the use of simpler random number distributions is a safe procedure which, in many cases, can save a significant amount of computer time.

In Sec. 2, we formulate the Langevin equation and its corresponding Fokker–Planck equation. From this we heuristically derive the standard Euler algorithm with the usual Gaussian distribution. The derivation is basically the historical reason for the widespread use of Gaussian random numbers. In Sec. 3, we introduce a broad class of distribution functions which can all be used in a numerical simulation. By a straightforward analytical consideration (which is not meant as a rigorous proof) we show weak convergence of the probability distribution of *sets of paths*, i.e., loosely spoken, in the limit $h \to 0$ the simulated probability to "choose" a path is the correct one. This means that all statistical properties are reproduced correctly in that limit, which is quite obvious since all statistical averages (single-time and multi-time) can be represented as a path integral. We think that this kind of approach is most natural and appropriate for the discussion of algorithms for the numerical integration of stochastic differential equations. Finally, in Sec. 4, we present numerical results for mean first exit time problems in simulations of the Wiener process (simple diffusion), the Ornstein–Uhlenbeck process (Brownian particle subject to a harmonic force) and the diffusion over a barrier in a Ginzburg–Landau type potential, using both Gaussian and uniform random numbers. In accordance with Strittmatter[5,6] we observe a $\sqrt{h}$ convergence behavior of the mean first exit time, a quantity which is very sensitive to the trajectories themselves.

2. The Fokker–Planck Process and the Standard Euler Algorithm

Our starting point is the stochastic differential equation

$$\dot{x} = f(x, t) + \sigma(x, t)\, \eta(t)\,. \tag{2.1}$$

f describes the deterministic drift, σ the diffusion. $\eta(t)$ is a stochastic force with the properties

$$\langle \eta(t) \rangle = 0\,, \tag{2.2}$$

$$\langle \eta(t)\eta(t') \rangle = 2\delta(t - t')\,, \tag{2.3}$$

$$\langle \eta(t_1)\eta(t_2)\dots\eta(t_{2n})\rangle = 2^n \sum_P \delta(t_{i_1} - t_{i_2}\dots\delta(t_{i_{2n-1}} - t_{i_{2n}}) \tag{2.4}$$

and

$$\langle \eta(t_1)\eta(t_2)\dots\eta(t_{2n+1})\rangle = 0\,. \tag{2.5}$$

In (2.4), the sum has to be performed over all permutations that lead to different expressions for $\delta(t_{i_1} - t_{i_2})\dots\delta(t_{i_{2n-1}} - t_{i_{2n}})$ (see e.g. Ref. 1). We choose the Itô interpretation of (2.1).

For convenience of notation, we restrict the discussion to one-dimensional processes. The generalization to several dynamical variables is straightforward.

The Markov process may alternatively be described by the conditional probability density $P(x, t|x_0, t_0)$. $P(x, t|x_0, t_0)\,dx$ is the probability for the random variable x having at time t a value in an interval of length dx under the condition that x had the value x_0 at time t_0. Obviously,

$$P(x, t_0|x_0, t_0) = \delta(x - x_0)\,. \tag{2.6}$$

The probability density $W(x, t)$ for the stochastic variable having the value x at time t can then be written as

$$W(x, t) = \int P(x, t|x_0, t_0)W(x_0, t_0)\,dx_0\,. \tag{2.7}$$

By the standard Kramers–Moyal expansion[1,2] it can be shown that P satisfies the following equation of motion:

$$\frac{\partial}{\partial t}P(x, t|x_0, t_0) = \sum_{n=1}^{\infty}\left(-\frac{\partial}{\partial x}\right)^n \left(D^{(n)}(x, t)P(x, t|x_0, t_0)\right), \tag{2.8}$$

where $D^{(n)}$ is given by

$$\begin{aligned} D^{(n)}(x, t) &= \frac{1}{n!}\lim_{\tau\to 0}\frac{1}{\tau}\,\langle (x'(t+\tau) - x'(t))^n\rangle\,|_{x'(t)=x} \\ &= \frac{1}{n!}\lim_{\tau\to 0}\frac{1}{\tau}\int (x' - x)^n P(x', t+\tau|x, t)\,dx'\,. \end{aligned} \tag{2.9}$$

Equations (2.8), (2.9) hold for an arbitrary Markov process. The properties (2.4), (2.5) of the noise ensure that in our case, the Fokker–Planck process, $D^{(n)}$ vanishes for $n > 2$. For the drift and diffusion coefficients $D^{(1)}$ and $D^{(2)}$ one obtains in the Itô interpretation[1,2]

$$D^{(1)}(x, t) = f(x, t)\,, \tag{2.10}$$

$$D^{(2)}(x, t) = \sigma(x, t)^2\,. \tag{2.11}$$

By (2.7) one immediately sees that $W(x, t)$ also obeys the Fokker–Planck equation.

A simulation is performed if an exact analytical solution is unknown. However, one may derive an approximate solution valid for short times. Assuming that drift and diffusion coefficients $D^{(1)}$ and $D^{(2)}$ are continuous functions of x and t, one may make use of the continuity of the trajectories and replace $D^{(1)}$ and $D^{(2)}$ by constants. The approximate Fokker–Planck equation, valid for small $t - t_0$, then becomes

$$\begin{aligned}\frac{\partial}{\partial t}P(x, t|x_0, t_0) = &-D^{(1)}(x_0, t_0)\frac{\partial}{\partial x}P(x, t|x_0, t_0) \\ &+ D^{(2)}(x_0, t_0)\frac{\partial^2}{\partial x^2}P(x, t|x_0, t_0)\end{aligned} \tag{2.12}$$

with the standard initial condition (2.6). As (2.12) is linear, it can be easily solved to yield the so-called "short-time propagator"

$$\begin{aligned}&P_S(x, t|x_0, t_0) = \\ &\left[4\pi D^{(2)}(x_0, t_0)(t - t_0)\right]^{-1/2} \exp\left(-\frac{(x - x_0 - D^{(1)}(x_0, t_0)(t - t_0))^2}{4D^{(2)}(x_0, t_0)(t - t_0)}\right),\end{aligned} \tag{2.13}$$

which is a Gaussian distribution. The corresponding Euler algorithm with timestep h then consists of the following recipe: If $x_0 = x(t_0)$ already has been generated, then generate $x = x(t_0 + h)$ according to the distribution (2.13):

$$x(t_0 + h) = x(t_0) + f(x_0, t_0)h + \sigma(x_0, t_0)\sqrt{2h}\, r\,, \tag{2.14}$$

where r is a Gaussian random variable with zero mean and unit variance. f and σ are the drift and diffusion terms of the Langevin equation (cf. Eqs. (2.10), (2.11)). The random variable $\sqrt{2h}\, r$ corresponds to $\int_0^h \eta(t)\, dt$ in the Langevin equation.

3. Use of Arbitrary Distributions

It is known that short-time propagators of the Fokker–Planck equation are not unique in general.[7,8] Indeed, the formula (2.9) suggests that *any* short-time propagator (i.e., algorithm) should be correct in the limit $h \to 0$ that has the property

$$\frac{1}{n!}\lim_{h\to 0}\frac{1}{h}\langle(\Delta x)^2\rangle = \frac{1}{n!}\lim_{h\to 0}\frac{1}{h}\int (x - x_0)^n P_S(x, t_0 + h|x_0, t_0)\, dx = D^{(n)}(x_0, t_0) \tag{3.1}$$

for all n. Later, we will give an argument that this is correct. The propagator (2.13), however, is not the only function that satisfies (3.1). A straightforward generalization can, e.g. be done by a scaling ansatz. Suppose an arbitrary function $F \geq 0$ be given having the properties

$$\int_{-\infty}^{\infty} F(x)\, dx = 1, \quad \int_{-\infty}^{\infty} xF(x)\, dx = 0, \quad \int_{-\infty}^{\infty} x^2 F(x)\, dx = 1\,, \tag{3.2}$$

all higher moments existing. F can be, e.g. a Gaussian, a uniform distribution, a sum of two delta functions peaked at ± 1, etc. One then easily verifies that (3.1) as

well as the initial condition (2.6) holds for

$$P_S(x, t_0 + h|x_0, t_0) = \frac{1}{\sqrt{2D^{(2)}(x_0, t_0)h}} F\left(\frac{x - x_0 - D^{(1)}(x_0, t_0)h}{\sqrt{2D^{(2)}(x_0, t_0)h}}\right). \tag{3.3}$$

The actual calculation is performed in Appendix A. From now on, the term "arbitrary distribution function" shall denote a short-time propagator normalized to unity that satisfies the initial condition (2.6) and the relations (3.1).

An intuitive argument why only the first two moments of the short-time propagator enter can be found in the classical paper by Chandrasekhar.[9] Describing the stochastic force by the physical picture of a large Brownian particle colliding stochastically with small surrounding particles, one must view $\int_0^h \eta(h)\, dt$ as the (additive) result of a large number of collisions, even for arbitrarily small h. (If one reaches a time scale where this is physically no longer valid, the Markov description of the dynamics is no longer correct.) Though the single collision has an unknown distribution, $\int_0^h \eta(t)\, dt$ must be a Gaussian random variable because of the Central Limit Theorem. In this limiting distribution only the first and second moment survive. By simply reverting this argument, it is obvious why one is allowed to choose an arbitrary short-time propagator: As the deterministic displacement scales as h, but the stochastic displacement as $\sqrt{h}$, the latter dominates in the limit of small timesteps. If h is sufficiently small, then lots of stochastic displacements have occurred before a significant deterministic drift has happened. So, on the time scale of the deterministic drift the distribution of the stochastic displacements may be regarded as Gaussian anyway.

We now want to give a more formal argument why every simulated short-time propagator satisfying (3.1) indeed yields the correct distribution of trajectories in the limit $h \to 0$. To this end, we consider the ensemble of paths starting at time $t = 0$ at $x = 0$ and ending somewhere at time $t = \tau = Nh$. For $t = nh$, $n = 1, 2, \ldots$ we choose intervals I_n (which can be very small). By requiring $x(nh) \in I_n$ we select a subset out of the set of all paths. The true probability measure of this subset is

$$\begin{aligned} W^t(h) = &\int_{I_N} dx_N \int_{I_{N-1}} dx_{N-1} \ldots \int_{I_1} dx_1 \\ &P^t(x_N, Nh|x_{N-1}, (N-1)h) \ldots P^t(x_1, h|0, 0)\,, \end{aligned} \tag{3.4}$$

where P^t stands for the true solution of the Fokker–Planck equation. Likewise, the simulated probability measure of this subset of paths is $W^s(h)$, where P^t has been replaced by the approximation short-time propagator P^s of the simulation. The method converges if for arbitrary choice of the I_n

$$\lim_{h \to 0} |W^s(h) - W^t(h)| = 0\,. \tag{3.5}$$

By adding $N-1$ zeros and using the triangle inequality, we have

$$\begin{aligned}|W^s(h)-W^t(h)| \leq \\ &\int_{I_N} dx_N \ldots \int_{I_1} dx_1 P_N^s P_{N-1}^s \ldots P_2^s |P_1^s - P_1^t| + \\ &\int_{I_N} dx_N \ldots \int_{I_1} dx_1 P_N^s P_{N-1}^s \ldots P_3^s |P_2^s - P_2^t| P_1^t + \ldots \\ &\int_{I_N} dx_N \ldots \int_{I_1} dx_1 |P_N^s - P_N^t| P_{N-1}^t \ldots P_1^t ,\end{aligned} \tag{3.6}$$

where the abbreviation

$$P_n := P(x_n, nh|x_{n-1}, (n-1)h) \tag{3.7}$$

has been introduced. The Fourier representation of P_n is written as

$$P(x_n, nh|x_{n-1}, (n-1)h) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ \exp(-ik(x_n - x_{n-1}))\tilde{P}(k; x_{n-1}, h)\,. \tag{3.8}$$

The moments of P_n are related to the Taylor coefficients of $\tilde{P}$:

$$\tilde{P}(k; x_{n-1}, h) = \sum_{\nu=0}^{\infty} \frac{(ik)^\nu}{\nu!}\mu_\nu(x_{n-1}, h) \tag{3.9}$$

with

$$\mu_\nu(x_{n-1}, h) = \int_{-\infty}^{\infty} dx_n (x_n - x_{n-1})^\nu P(x_n, nh|x_{n-1}, (n-1)h)\,. \tag{3.10}$$

Hence,

$$P_n^s - P_n^t = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ \exp(-ik(x_n - x_{n-1}))\sum_{\nu=0}^{\infty}\frac{(ik)^\nu}{\nu!}(\mu_\nu^s - \mu_\nu^t)\,. \tag{3.11}$$

Because of the premise (3.1), $\mu_\nu^s - \mu_\nu^t$ vanishes faster than linearly as $h \to 0$, $\mu_\nu^s - \mu_\nu^t = o(h)$. Hence, $P_n^s - P_n^t = o(h)$. On the other hand, the number of terms appearing in (3.6) is $N = \tau/h$. Therefore, (3.1) indeed assures convergence.

4. Numerical Results

In order to check the influence of the details of the distribution function on the convergence behavior, we performed Brownian dynamics simulations on three simple systems, the Wiener process

$$\frac{\partial P}{\partial t} = L_{FP}(x)P = \frac{1}{2}\frac{\partial^2 P}{\partial x^2}\,, \tag{4.1}$$

the Ornstein–Uhlenbeck process

$$\frac{\partial P}{\partial t} = L_{FP}(x)P = \left(\frac{\partial}{\partial x}x + \frac{1}{2}\frac{\partial^2}{\partial x^2}\right)P\,, \tag{4.2}$$

and a "Ginzburg–Landau" process

$$\frac{\partial P}{\partial t} = L_{FP}(x)P = \left(\frac{\partial}{\partial x}(x^3 - x) + D\frac{\partial^2}{\partial x^2}\right)P\,, \tag{4.3}$$

where we use $D = 0.1$ in our simulation.

For these processes we calculated mean first exit times. These are defined as follows: Suppose that the stochastic variable x has a starting value $x = x_0$ at time $t = 0$, and that an interval I is given around x_0. For a given trajectory, the first exit time is the time that passes until x for the first time has a value *not* in I. The mean first exit time $T(x_0)$ then results from averaging over all trajectories.

The Wiener and the Ornstein–Uhlenbeck processes were studied using the Euler algorithm and five different timesteps (h = 0.0005, 0.001, 0.005, 0.01, 0.05) and both Gaussian and uniform random numbers. We generated 10^6 trajectories for each system, timestep and type of random numbers, and calculated the mean first exit time for the escape beyond $|x| = 1$ starting at $x = 0$. In the case of the Ginzburg–Landau double well potential we asked for the escape time out of one of the symmetric minima at $x = \pm 1$ over the barrier at $x = 0$. We again used the Euler algorithm and six timesteps (same as before, additionally $h = 0.0025$) and generated $5 \cdot 10^5$ paths for both types of random numbers. The simulations were run on the Cray at the HLRZ Jülich using a fully vectorized program. Even for the most complicated case, the Ginzburg–Landau process, the simulation using Gaussian random numbers (Box–Muller algorithm[10]) needed about four times as much CPU time as the program that used uniform ones.

In order to compare our results with exact values, we make use of the fact that the mean first exit time $T(x)$ for the escape out of an interval $[a, b]$ obeys the differential equation[1,2]

$$L_{LP}^{\dagger}T(x) + 1 = 0 \tag{4.4}$$

with the boundary conditions

$$T(a) = T(b) = 0 \tag{4.5}$$

for the case of absorbing boundaries (Wiener process and Ornstein–Uhlenbeck process) and

$$T(0) = 0, \quad \frac{d}{dx}T(x) \overset{x\to-\infty}{\longrightarrow} 0 \tag{4.6}$$

for an absorbing boundary at $x = 0$ and a reflecting one at $x = -\infty$ (Ginzburg–Landau process).

In (4.4), $L_{FP}^{\dagger}$ denotes the adjoint operator of the Fokker–Planck operator which is

$$L_{FP}^{\dagger} = \frac{1}{2}\frac{\partial^2}{\partial x^2} \tag{4.7}$$

in the case of the Wiener process,

$$L_{FP}^{\dagger} = -x\frac{\partial}{\partial x} + \frac{1}{2}\frac{\partial^2}{\partial x^2} \tag{4.8}$$

for the ornstein–Uhlenbeck process and

$$L_{FP}^{\dagger} = (x - x^3)\frac{\partial}{\partial x} + D\frac{\partial^2}{\partial x^2} \tag{4.9}$$

for the Ginzburg-Landau process.

For the Wiener process, one trivially obtains $T(x) = 1 - x^2$ and $T(0) = 1$. For the Ornstein–Uhlenbeck process, we solved (4.4), (4.5) numerically by a power series ansatz on a pocket calculator to obtain $T(0) = 1.44525$. In the case of the Ginzburg–Landau process the exact value for $T(-1)$ can be obtained by a Romberg integration[5,6] of the double integral representation of $T(x)$[1,2] or by a numerical integration of (4.4, 4.6) using a shooting procedure. For $D = 0.1$ both methods yield a value of $T(-1) = 30.82$.

The discretization error of T should (in leading order) be proportional to $\sqrt{h}$.[4–6] Furthermore, the data are subject to a statistical error due to the finite sample size. In the cases of the Wiener and Ornstein–Uhlenbeck process we estimated the error by

$$\sigma(T) = \frac{\sqrt{\langle T^2\rangle - \langle T\rangle^2}}{\sqrt{N}} \approx \frac{\langle T\rangle}{\sqrt{N}}, \tag{4.10}$$

where $\langle T\rangle$ is the simulation result for the mean first exit time and N is the number of generated paths. In the case of the Ginzburg–Landau process we explicitly sampled $\sigma(T)$. The extrapolation to timestep $h = 0$ was done by fitting a linear behavior in $\sqrt{h}$ to the data.[10] In two cases (Ginzburg–Landau with uniform random numbers, Ornstein–Uhlenbeck with Gaussian random numbers) we used all data points, whereas we omitted the largest time step in all other cases since the quality of the fit[10] decreased significantly if the data point was included. We ascribe this behavior to a $O(h)$–contribution. Table 1 gives our results, including the error of the extrapolated value calculated by the regression routine (one standard deviation). The raw data and the fitted straight lines are presented in Figs. 1–3.

Table 1. Results for mean first exit times.

Process	exact	uniform	Gauss
Wiener	1	0.999 ± 0.001	0.997 ± 0.001
Ornstein–Uhlenbeck	1.445	1.444 ± 0.002	1.444 ± 0.001
Ginzburg–Landau	30.82	30.85 ± 0.03	30.85 ± 0.04

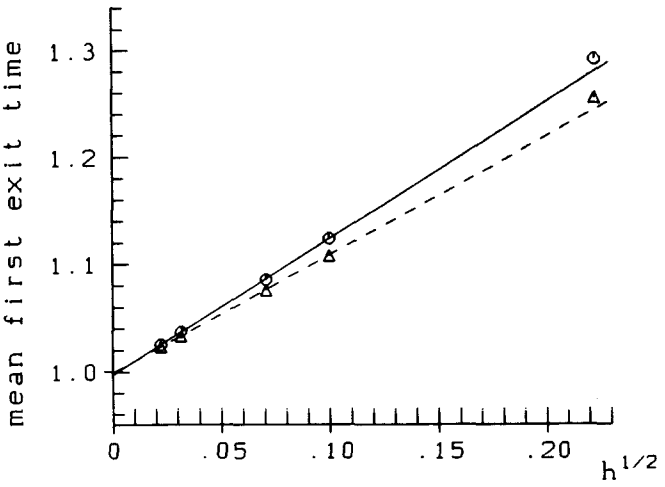

Fig. 1. This mean first exit time as a function of the square root of the discretization timestep for the Wiener process. Octagons denote Gaussian random numbers and triangles uniform ones. In all cases the symbol size exceeds the statistical error of the data. The straight lines are regression fits (see text).

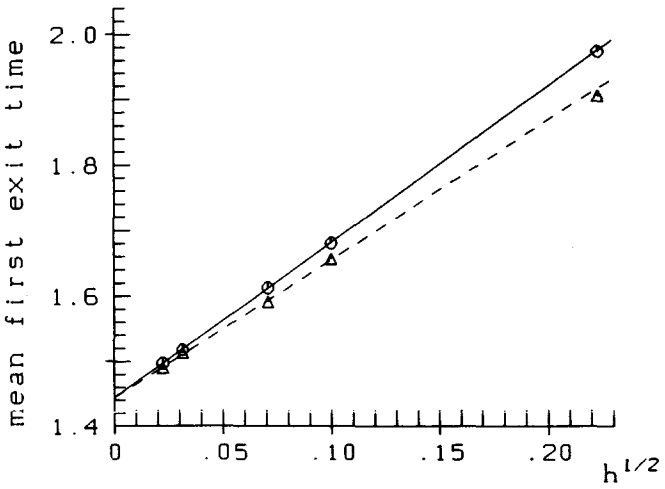

Fig. 2. Same as Fig. 1 for the Ornstein–Uhlenbeck process.

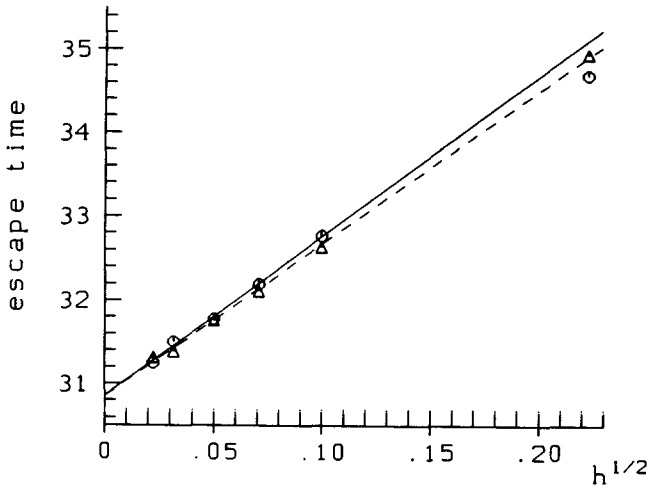

Fig. 3. Same as Fig. 1 for the Ginzburg–Landau process.

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Appendix A

In order to check that (3.3) satisfies (3.1) we have to compute the integrals

$$I_n := \int_{-\infty}^{\infty} (x - x_0)^n \frac{1}{\sqrt{2D^{(2)}(x_0, t_0)h}} F\left(\frac{x - x_0 - D^{(1)}(x_0, t_0)h}{\sqrt{2D^{(2)}(x_0, t_0)h}}\right) dx \tag{A.1}$$

to low orders of the timestep h. By the abbreviations

$$a := \sqrt{2D^{(2)}(x_0, t_0)} \tag{A.2}$$

and

$$b := \frac{D^{(1)}(x_0, t_0)}{a} \tag{A.3}$$

one has

$$I_n = \int_{-\infty}^{\infty} \frac{(x - x_0)^n}{a\sqrt{h}} F\left(\frac{x - x_0}{a\sqrt{h}} - b\sqrt{h}\right) dx\,. \tag{A.4}$$

Substituting

$$y := \frac{x - x_0}{a\sqrt{h}} - b\sqrt{h} \tag{A.5}$$

and expanding

$$(x - x_0)^n = (a\sqrt{h})^n (y + b\sqrt{h})^2 = (a\sqrt{h})^2 \sum_{k=0}^{n} \binom{n}{k} (b\sqrt{h})^k y^{n-k} \tag{A.6}$$

we find

$$I_n = a^n h^{n/2} \sum_{k=0}^{n} \binom{n}{k} b^k h^{k/2} \int_{-\infty}^{\infty} y^{n-k} F(y)\, dy\,. \tag{A.7}$$

We now use the properties (3.2) required for the function F. For $n = 0$, one obtains $I_0 = 1$. That means that the short-time propagator is correctly normalized. For $n = 1$, only $k = 1$ contributes: $I_1 = abh$. Hence,

$$\lim_{h \to 0} \frac{I_1}{h} = ab = D^{(1)}(x_0, t_0)\,. \tag{A.8}$$

For $n = 2$, only $k = 0$ and $k = 2$ contribute: $I_2 = a^2 h(1 + b^2 h)$, and

$$\frac{1}{2} \lim_{h \to 0} \frac{I_2}{h} = \frac{a^2}{2} = D^{(2)}(x_0, t_0)\,. \tag{A.9}$$

For $n \geq 3$, $I_n = O(h^{n/2})$, and hence

$$\frac{1}{n!} \lim_{h \to 0} \frac{I_n}{h} = 0\,. \tag{A.10}$$